Quantum rejection sampling

Maris Ozols
Martin Rötteler
Jérémie Roland

University of Waterloo
NEC Laboratories America
Université Libre de Bruxelles

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Introduction

- (Classical) rejection sampling
  - Algorithmic tool introduced by von Neumann (1951)
  - Can be used to sample from arbitrary distributions
  - Numerous applications:
    - ✱ Metropolis algorithm [MRRTT53]
    - ✱ Monte-Carlo simulations
    - ✱ optimization (simulated annealing)
    - ✱ etc...
- Quantum rejection sampling
  - Natural quantum analogue: probabilities ➜ amplitudes
  - New algorithmic tool
  - Applications:
    - ✱ Linear system of equations [HHL09]
    - ✱ Quantum Metropolis algorithm
    - ✱ Boolean hidden shift problem

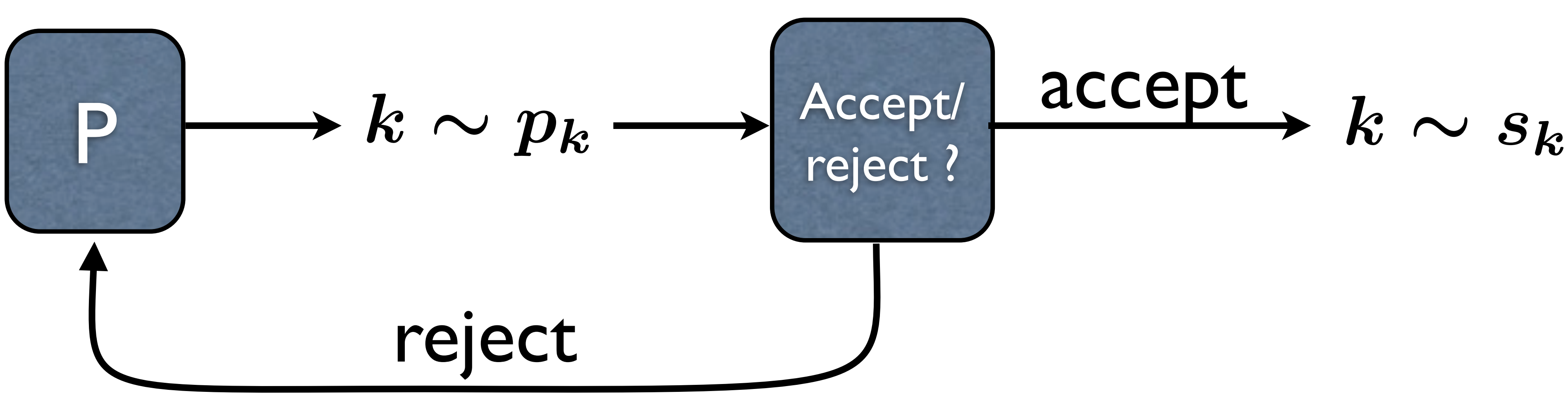
Classical resampling problem

Setup:

- P and S: two probability distributions

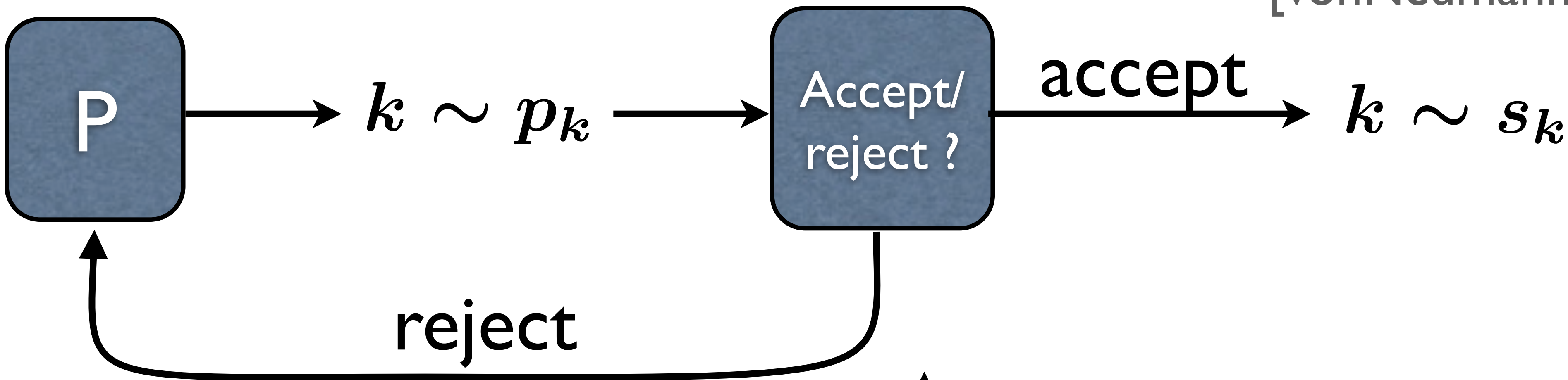
Resampling problem

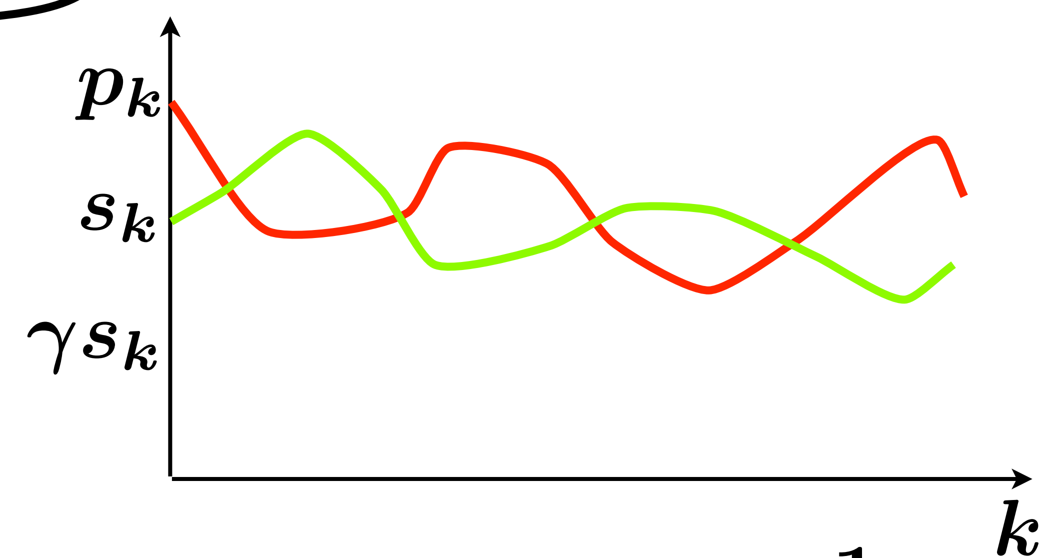
Given the ability to sample according to P, produce a sample distributed according to S.



Rejection sampling

[vonNeumann51]





- $\Pr[\text{accept } k] = \gamma \frac{s_k}{p_k}$
- $\gamma = \min_k \frac{p_k}{s_k}$
- Expected number of required samples: $T = \frac{1}{\gamma}$
- This is optimal [Letac75]
- Many applications in randomized algorithms

Quantum resampling problem

- Given access to a black box O_ξ preparing a state

$$|\pi^\xi\rangle = \sum_k \pi_k |\xi_k\rangle |k\rangle$$

known amplitudes

unknown states

- Prepare the state

$$|\sigma^\xi\rangle = \sum_k \sigma_k |\xi_k\rangle |k\rangle$$

different amplitudes

same states

- Question: How many calls to O_ξ are necessary?

- Tool: Query complexity

Classical query complexity

- Function $f(x)$, where $x = (x_1, \ldots, x_n)$
- Oracle $O_x : i \rightarrow x_i$
- Goal: Compute $f(x)$ given black-box access to O_x

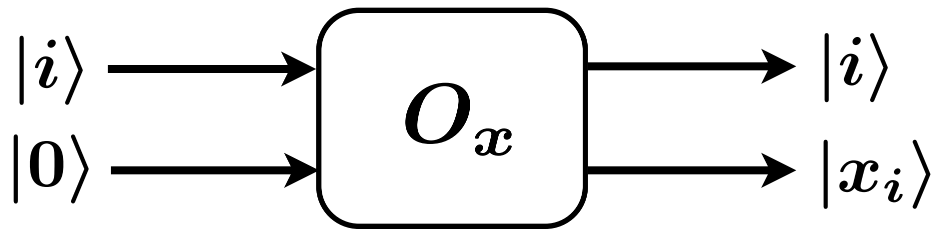
Randomized query complexity $R_\varepsilon(f)$

Minimum # calls to O_x necessary to compute $f(x)$ with success probability $(1 - \varepsilon)$

Quantum query complexity

Different quantum extensions:

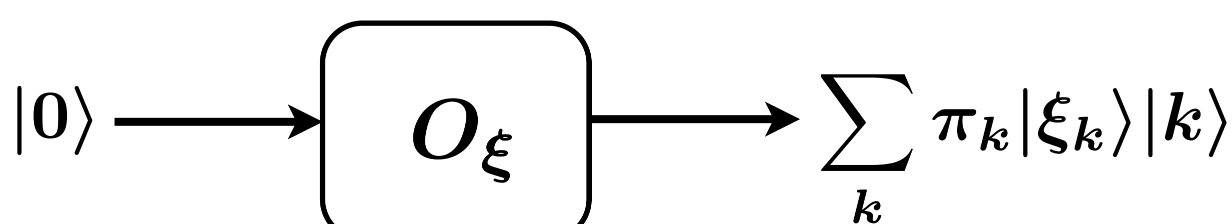
1. Can query O_x in superposition $\Rightarrow Q_\varepsilon(f) \leq R_\varepsilon(f)$



2. Instead of computing a function $f(x)$, generate a quantum state $|\psi_x\rangle$

3. Oracle O_ξ is a unitary that hides the label ξ in a non-explicit way

Example: Quantum resampling



Quantum state generation

- Set of quantum states $\Psi = \{|\psi_\xi\rangle : \xi \in \mathcal{X}\}$
- Set of oracles $\mathcal{O} = \{O_\xi : \xi \in \mathcal{X}\}$
- Quantum state generation problem $\mathcal{P}$ defined by $(\Psi, \mathcal{O})$
- Goal: Generate $|\psi_\xi\rangle$ given black-box access to O_ξ

Quantum query complexity $Q_\varepsilon(\mathcal{P})$

Minimum # calls to O_ξ necessary to generate a state $\sqrt{1-\varepsilon}|\psi_\xi\rangle|\bar{0}\rangle + \sqrt{\varepsilon}|\mathrm{error}_\xi\rangle$

work space

Quantum rejection sampling

Need to change $\pi_k \to \sigma_k$.

- Use oracle O_ξ to create the original state

$$O_\xi|0\rangle = \sum_k \pi_k |\xi_k\rangle|k\rangle$$

Will be chosen later

- Use control-rotation on an ancilla qubit

$$|0\rangle \to \sum_k |\xi_k\rangle|k\rangle\left(\sqrt{|\pi_k|^2 - |\alpha_k|^2}|0\rangle + \alpha_k|1\rangle\right)$$

- If we measure the ancilla and obtain $|1\rangle$ ("accept"):

$$\frac{1}{\|\vec{\alpha}\|}\sum_k \alpha_k|\xi_k\rangle|k\rangle$$

- OK if $\vec{\alpha}$ is close to $\vec{\sigma}$, more precisely:

$$\frac{\vec{\sigma}\cdot\vec{\alpha}}{\|\vec{\alpha}\|} \geq \sqrt{1-\varepsilon}$$

Optimization

$$\sum_k |\xi_k\rangle|k\rangle\left(\sqrt{|\pi_k|^2 - |\alpha_k|^2}|0\rangle + \alpha_k|1\rangle\right)$$

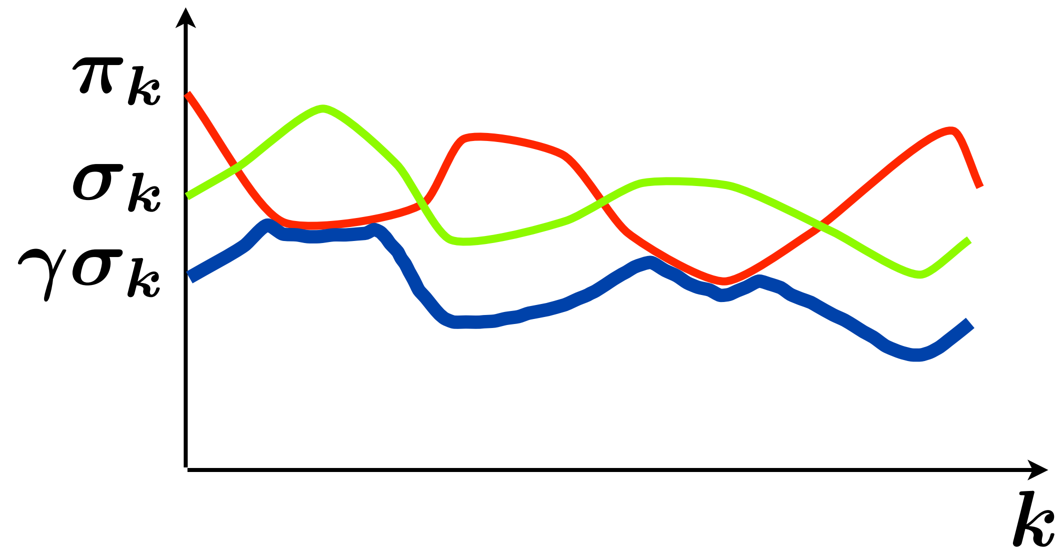
- We measure $|1\rangle$ ("accept") with probability $\|\vec{\alpha}\|^2$
- Naive approach: repeat $O(1/\|\vec{\alpha}\|^2)$ times
- Using amplitude amplification: reduce to $O(1/\|\vec{\alpha}\|)$ [BrassardHøyerMoscaTapp00]
- Optimizing $\vec{\alpha}$: Semidefinite program

Maximize $\|\vec{\alpha}\|$ subject to $0 \leq \alpha_k \leq \pi_k \quad \forall\, k$

$$\frac{\vec{\sigma}\cdot\vec{\alpha}}{\|\vec{\alpha}\|} \geq \sqrt{1-\varepsilon}$$

Optimal solution

- Let $\alpha_k(\gamma) = \min\{\pi_k, \gamma\sigma_k\}$



- We take $\bar{\gamma} = \max \gamma$ such that $\dfrac{\vec{\sigma} \cdot \vec{\alpha}(\gamma)}{\|\vec{\alpha}(\gamma)\|} \geq \sqrt{1 - \varepsilon}$
- We can prove that this leads to an optimal algorithm

Matching lower bound uses automorphism principle with $G = \mathbb{Z}_2^n \times U(N-1)$

Theorem

$$Q_\varepsilon(\mathrm{QSampling}_{\vec{\pi} \to \vec{\sigma}}) = \Theta(1/\|\vec{\alpha}(\bar{\gamma})\|)$$

Applications

- Linear system of equations [HHL09]
  - QRS was used implicitly
- Quantum Metropolis algorithm
  - Improvement on the original algorithm [TOVPV11]
- Boolean hidden shift problem
  - New algorithm!

Linear system of equations

[HHL09]

Setup:

- Invertible $d \times d$ matrix A
- Vector $|b\rangle \in \mathbb{C}^d$

can be assumed Hermitian

Quantum linear equations problem

Prepare the state $|x\rangle$ such that

$$A|x\rangle = |b\rangle$$

Main idea: use quantum phase estimation (QPE) [Kitaev95,CEMM97]

+ quantum rejection sampling (QRS)

Algorithm [HarrowHassidimLloyd09]

$$A|x\rangle = |b\rangle \Leftrightarrow |x\rangle = A^{-1}|b\rangle$$

- Let $|b\rangle = \sum_k b_k|\psi_k\rangle$, where
  - $|\psi_k\rangle$ are the eigenstates of A
  - λ_k are the corresponding eigenvalues
- Use QPE to prepare $|b\rangle = \sum_k b_k|\psi_k\rangle|\lambda_k\rangle$
- Use QRS to get $\sum_k b_k\lambda_k^{-1}|\psi_k\rangle|\lambda_k\rangle$
  - Known amplitude (ratios): λ_k^{-1}
  - Unknown states: $|\psi_k\rangle$
- Undo phase estimation to obtain

$$|x\rangle = \sum_k b_k\lambda_k^{-1}|\psi_k\rangle = A^{-1}|b\rangle$$

Quantum Metropolis algorithm

Setup:

- Hamiltonian H
  - Eigenstates $|\psi_k\rangle$
  - Eigenenergies E_k
- Inverse temperature β

Metropolis sampling problem

Prepare the thermal state $\sum_k p_k|\psi_k\rangle\langle\psi_k|$, where $p_k \sim \exp(-\beta E_k)$ is the Gibbs distribution

Classical solution

[MRRTT53]

- If H is diagonal (=classical)
  - Eigenstates $|\psi_k\rangle$ are known
  - Eigenenergy E_k can be efficiently computed from $|\psi_k\rangle$
- Start from a random $|\psi_k\rangle$

e.g., spin flip

- Apply a "kick" to get another $|\psi_l\rangle$
- Compute the energies E_k and E_l
  - If $E_l \leq E_k$, accept the move
  - If $E_l > E_k$, accept only with probability $\exp(\beta(E_k - E_l))$
- Repeat

Quantum Metropolis algorithm

- If H is not diagonal (=quantum)
  - Eigenstates $|\psi_k\rangle$ and eigenergies E_k are not known to start with
  - But: we can project onto the $|\psi_k\rangle$-basis and get the corresponding E_k by using quantum phase estimation (QPE).
- Prepare a random $|\psi_k\rangle$ using QPE (and record E_k)
- Apply a "kick" (random unitary gate)
- Use QPE to project on another $|\psi_l\rangle$ (and record E_l)
- Compare the energies E_k and E_l
  - If $E_l \leq E_k$, accept the move
  - If $E_l > E_k$, accept only with probability $\exp(-\beta(E_l - E_k))$

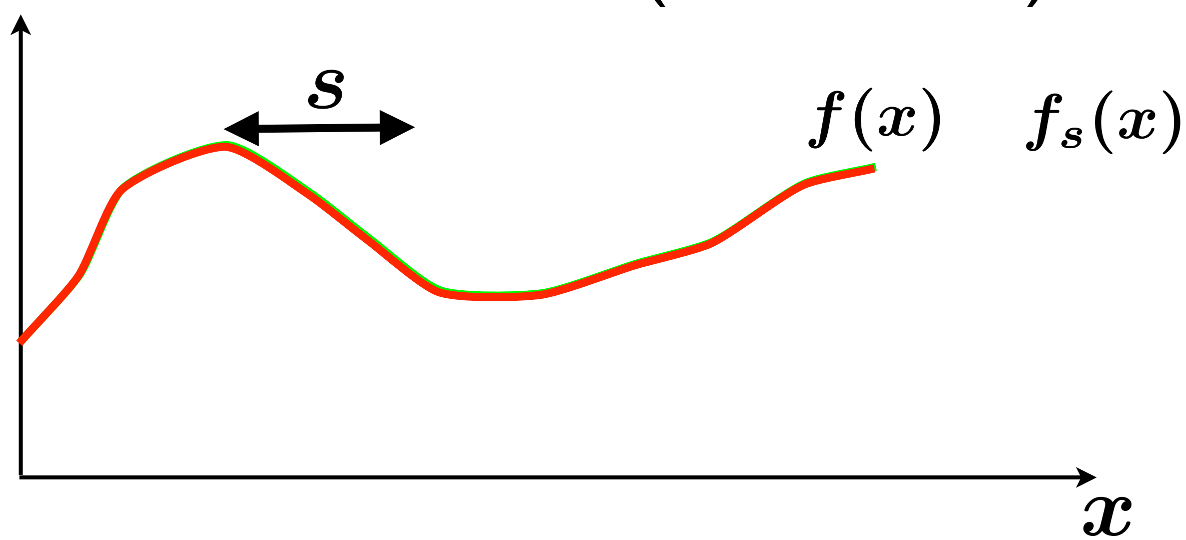
Quantum Metropolis algorithm

- Problem:
  - Rejected moves require to revert the state from $|\psi_l\rangle$ to $|\psi_k\rangle$
  - We cannot keep a copy of $|\psi_k\rangle$ (requires to clone an unknown state!)
- Two solutions:
  - Temme *et al.* [TOVPV11] propose a "rewinding" technique to revert to $|\psi_k\rangle$, based on a series of projective measurements.
  - Use quantum rejection sampling! Equivalent to amplifying accepted moves, therefore avoiding having to revert moves at all.

Boolean hidden shift

Setup:

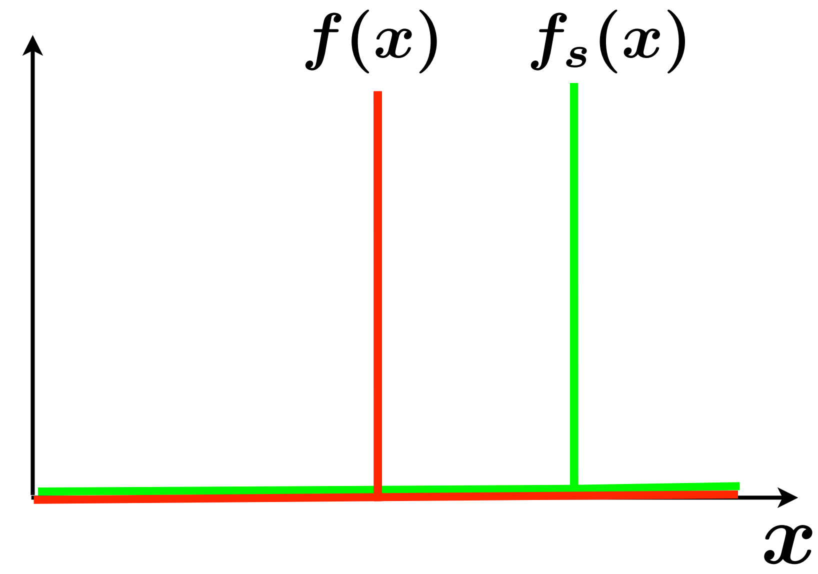
- $f(x)$:(known) Boolean function
- $f_s(x) = f(x+s)$, with an (unknown) shift $s \in \{0,1\}^n$



Boolean hidden shift problem

Given black-box access to $f_s(x)$,
find the hidden shift s

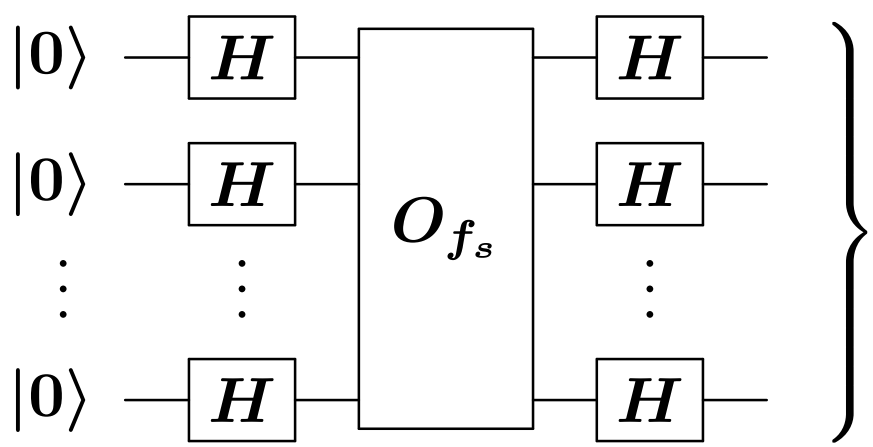
Special cases



- Delta function $f(x) = \delta_{xx_0}$
  - = Grover's search problem
  - Requires $\Theta(\sqrt{2^n})$ queries [Grover96]
- Bent functions
  - = Functions with flat Fourier spectrum
  - Can be solved with 1 query! [Rötteler10]
- What about other functions???

New algorithm based on QRS

- Use the following circuit, where
  - H is the Hadamard transform
  - O_{f_s} is the black box for f_s, acting as $O_{f_s}|x\rangle = (-1)^{f_s(x)}|x\rangle$



$$\sum_w (-1)^{w \cdot s} \hat{f}(w)|w\rangle$$

- Use QRS to produce the state $\frac{1}{\sqrt{2^n}} \sum_w (-1)^{w \cdot s}|w\rangle$
  - Known amplitudes = Fourier coefficients $\hat{f}(w)$
  - Unknown "states" = phases $(-1)^{w \cdot s}$
- Use a final Fourier transform $H^{\otimes n}$ to get $|s\rangle$

Wrap-up

- Rejection sampling has found many applications in classical computing
- Quantum rejection sampling could be as useful for quantum computing!
- Example: 3 diverse applications
  - Linear system of equations [HarrowHassidimLloyd09]
  - Quantum Metropolis algorithm
  - Boolean hidden shift problem

Outlook

- Other applications
  - Amplifying QMA witnesses [MarriottWatrous05,NagajWocjanZhang09]
  - Preparing PEPS states [SchwarzTemmeVerstraete11]
  - ???
- Adversary method for this extend model of quantum query complexity?
  - Non-trivial error dependence
  - Infinite-size adversary matrices

Support: